MULTIFLUID ALGORITHMS FOR EULERIAN FINITE DIFFERENCE METHODS

P. COLELLA*, H. M. GLAZ† AND R. E. FERGUSON‡

Abstract. A multifluid extension of the operator–split second–order Eulerian Godunov method is constructed; in addition to avoiding a Lagrange plus remap formulation, the resulting method is shown to satisfy the property that pressure equilibrium among the fluid components is maintained to leading order in the absence of strong shocks. A relaxation scheme which restores pressure equilibrium is introduced to handle such interactions. The multifluid algorithm is in the class of volume–of–fluid methods; the SLIC representation for subgrid structure is used here. Another important result derived here is that the multifluid system of PDE's is hyperbolic and has a natural physical interpretation. Computational results are presented which show that the new algorithm retains the high resolution, accuracy and stability properties of the basic single fluid method. Finally, the single fluid method has been modified with the result that it is more efficient as well as more robust with respect to wide variations in the equation–of–state.

1. Introduction. We present a volume-of-fluid type method for the numerical calculation of compressible flow problems in which the fluid is made up of a number of thermodynamically distinct materials separated by sharp interfaces. In this approach, a standard finite difference representation of the solution is augmented by cell-centered values for the thermodynamic quantities: ρ^α, e^α, ΔV^α, are the density, internal energy, and partial volume occupied by the α^{th} fluid in each zone, $\alpha = 1, \ldots, n_f$. The evolution of this representation can be thought of as consisting of two parts. One is the effective Lagrangian dynamics—the accelerations, compressions, and work done on the multifluid representation—which is computed under the assumption that the various fluid components are in pressure equilibrium with one another in each cell, and that each cell has a single velocity. From a physical point of view, the assumption of pressure equilibrium is not unreasonable, since the pressure is continuous across a contact discontinuity. The requirement that the cell has a single velocity is not an appropriate one in more than one dimension, since slip can be generated at a fluid interface. Thus, jumps in the thermodynamic variables across the interface are tracked, while the jump in tangential velocity is

*Mechanical Engineering Department, University of California, Berkeley, California 94720. The support of the Applied Mathematical Sciences Program of the U.S. Department of Energy at the Lawrence Livermore National Laboratory under Contract W–7405–Eng–48; of the Army Research Office under Grant DAALO3-88-K-0197; and of a National Science Foundation Presidential Young Investigator Award ASC–8958522, is gratefully acknowledged.

†Department of Mathematics, University of Maryland, College Park, Maryland 20742. The support of the National Science Foundation under Grant DMS-8703971; of the Applied Mathematical Sciences Program of the U.S. Department of Energy at the Courant Institute of Mathematical Sciences under Grant DE–FG02–88ER25053; and of the Defense Nuclear Agency under Contract DNA001–87–0303 is gratefully acknowledged.

‡Information and Mathematical Sciences Branch, Naval Surface Warfare Center, White Oak, Silver Spring, Maryland 20903. The support of the Defense Nuclear Agency, MIPR 90–567 is gratefully acknowledged.

captured using the underlying conservative finite difference method. The other part of the evolution is the motion of the fluid interface through the finite difference grid. This is done by reconstructing locally the interface geometry from the fractional volumes, and transporting material along streamlines defined by the single fluid velocities. Multifluid methods have been in use for some time [8,15,17,26] and have been quite effective in representing complicated multifluid configurations undergoing large distortions.

We introduce two innovations into this class of algorithms. The first one concerns the effective Lagrangian dynamics of the multifluid cells. A formulation of this dynamics is derived which is thermodynamically consistent in the following sense: if the various fluid components in a cell are in pressure equilibrium, then they remain so to leading order in the truncation error, assuming that the pressure gradients and compressions are finite. Since that assumption will occasionally be violated – for example, when a shock crosses a material interface – a relaxation scheme to restore pressure equilibrium in multifluid cells is also introduced. The second innovation is the coupling of this method to an operator-split second-order Eulerian Godunov method. In previous multifluid algorithms, the conceptual division into two parts was used literally as the basis for the design of the algorithm, with the underlying single-fluid algorithm having to be formulated as a Lagrangian step followed by a remap. In the approach taken here, the underlying difference algorithm is a conservative Eulerian predictor-corrector method which provides pressures and velocities at the cell edges as part of the flux calculation.

The basic ideas introduced here are presented in Section 2 in the context of constructing a multifluid Lagrangian method; in particular, our approach to partial volume updates, specific total energy redistribution over the fluid components and the pressure equilibrium algorithm during a time step can be easily understood in Lagrangian coordinates. The corresponding Eulerian algorithm is presented in Section 3. Our derivation begins at the PDE level in the sense that an effective multimaterial Eulerian dynamics is derived from physical principles along with the assumptions underlying the applicability of a volume–of–fluid approach. The resulting equations are formally derived in Appendix A wherein they are also shown to be hyperbolic in a natural way. Appendices B and C contain the new version of the underlying single fluid second–order Eulerian Godunov scheme and the SLIC fluid interface reconstruction algorithm used in our computations, respectively. The results of our calculations are presented in Section 4 and we summarize our conclusions in Section 5.

2. Lagrangian Dynamics and Thermodynamic Consistency.

A 1D Lagrangian multifluid algorithm (or a Lagrangian step of a 1D Lagrange + remap formulation of a multifluid Eulerian calculation) is developed in this section. In Lagrangian coordinates, the primary dependent variables for a single fluid problem are $(\tau, u, E)^t$, the specific volume, velocity and specific total energy of the gas. The independent variables are the time t, and a Lagrangian mass coordinate m. Additionally, it is assumed that the physical space coordinate system has a generalized volume coordinate arising from,

e.g., cylindrical or spherical geometry. Thus, a spatial coordinate x and functions $V(x)$, $A(x) = dV/dx > 0$ of the spatial coordinate specify the geometry. The location in space of a particle with mass coordinate m is given by $x(m,t)$, $\frac{d}{dt}(x(m,t)) = u(m,t)$. Given x(m,t), the functions $V(m), A(m) = V(x(m,t)), A(x(m,t))$ can be obtained.

In terms of these variables, the equations of gas dynamics are:

$$\begin{aligned} &\frac{\partial \tau}{\partial t} - \frac{\partial Au}{\partial m} = 0 \\ &\frac{\partial u}{\partial t} + A\frac{\partial p}{\partial m} = 0 \\ &\frac{\partial E}{\partial t} + \frac{\partial Aup}{\partial m} = 0\,. \end{aligned} \tag{2.1}$$

Here, p is the thermodynamic pressure of the gas, $p = p(\rho, e)$, $\rho = \tau^{-1}$ is the density and $e = E - \frac{1}{2}u^2$ is the specific internal energy of the gas. The speed of sound of the gas is a function of the thermodynamic quantities and is given by $c^2 = pp_e/\rho^2 + p_\rho$. It is standard to use the form $c^2 = \Gamma p/\rho, \Gamma = \Gamma(\rho, e)$. Finally, the volume coordinate can be expressed directly in terms of the other dependent variables:

$$V(x(m,t)) = \int_{m_0}^{m} \tau(m',t)\, dm'\,,$$

where m_0 is some constant independent of t. Physically, $V(x(m,t))$ is the volume occupied by the fluid contained between the mass coordinates m and m_0.

An underlying single-fluid Lagrangian algorithm of a predictor–corrector type is assumed given, i.e., a scheme which, given τ^n, u^n, E^n, the solution at the old time, produces $u_{j+1/2}$, $p_{j+1/2}$ at the edges of cells to update the conserved quantities:

$$\begin{aligned} \tau_j^{n+1} &= \tau_j^n - \frac{\Delta t}{\Delta m_j}\,[Au]_j \\ u_j^{n+1} &= u_j^n + \overline{A}_j \frac{\Delta t}{\Delta m_j}\,[p]_j \\ E_j^{n+1} &= E_j^n + \frac{\Delta t}{\Delta m_j}\,[Aup]_j\ , \end{aligned} \tag{2.2}$$

where we denote by $[q]_j = q_{j-1/2} - q_{j+1/2}$, the jump in edge-centered values across a cell, $\overline{q}_j = \frac{1}{2}(q_{j+1/2} + q_{j-1/2})$ and $u_{j+1/2}$, $p_{j+1/2}$ are obtained from some finite difference procedure. In the remainder of the paper, we will suppress the spatial subscript j in expressions such as (2.2) if there is no chance of confusion.

The primary dependent variables for a multifluid Lagrangian algorithm are $(\rho^{\alpha,n}, e^{\alpha,n}, \Delta V^{\alpha,n};\ \alpha = 1, \ldots, n_f)$ where $\Delta V^{\alpha,n}$ denotes the volume occupied by fluid α. Our algorithm consists of several steps. First, effective single fluid values for the conserved

quantities τ^n, E^n, and the derived cell-centered quantities p^n and the sound speed c^n, are constructed in each of the multifluid cells. Second, a single fluid algorithm is used to obtain $u_{j+1/2}$, $p_{j+1/2}$. It is assumed in this step that the effective cell-centered quantities in the previous step are sufficient for calculating the single fluid fluxes. Two examples of schemes for which this is true are certain forms of the two-step Richtmyer version of Lax-Wendroff, and the Godunov methods discussed in [27]. The final step of the algorithm distributes the flux differences over the various fluid components in each cell. This is done in such a way that the total mass, momentum, and energy of the system are conserved, and single-valuedness of the velocity and pressure equilibrium among the fluid components in each cell is maintained.

In the first step, it is assumed that p^n is given by $p^n = \hat{p}(\{p^{\alpha,n}, \Delta V^{\alpha,n}, \dots\}; \alpha = 1, \dots, n_f)$, where the values for the variables $p^{\alpha,n}$, $\Gamma^{\alpha,n}$ and the other thermodynamic variables for each fluid are obtained from the dependent variables $(\rho^{\alpha,n}, e^{\alpha,n}, \Delta V^{\alpha,n}; \alpha = 1, \dots, n_f)$ and the equations–of–state for the n_f fluids. It is required that the function $\hat{p}$ be a smooth function of its arguments; that $\hat{p}$ be independent of the variables associated with the α^{th} fluid if $\Delta V^{\alpha,n} = 0$; and that, if $p^{\alpha,n} = p_0$ independent of α, then $\hat{p} = p_0$. One example of such a function is $\hat{p} = \left(\sum_\alpha p^{\alpha,n} \Delta V^{\alpha,n}\right) / \sum_\alpha \Delta V^{\alpha,n}$, which has been used extensively in multifluid calculations; an alternative formulation is suggested below. The single fluid specific volume, specific total energy, and total mass of the cell are given by appropriate mass-weighted averages:

$$
\begin{aligned}
\Delta m^\alpha &= \Delta V^{\alpha,n} \rho^{\alpha,n}\,, \\
\Delta m &= \sum_\alpha \Delta m^\alpha\,, \\
\Delta V &= \sum_\alpha \Delta V^{\alpha,n}\,, \\
\tau &= \frac{\Delta V}{\Delta m} = \frac{1}{\rho}\,, \\
E &= \sum_\alpha \Delta V^{\alpha,n} \rho^{\alpha,n} E^{\alpha,n} \Big/ \Delta m\,.
\end{aligned}
\tag{2.3}
$$

In calculating the effective sound speed in a multifluid zone, a relationship of the form

$$
-\Gamma \frac{\delta V}{\Delta V} = \frac{\delta p}{p}
\tag{2.4}
$$

is sought, where ΔV is the total volume of the zone, and δV and δp are arbitrary small increments in the total volume and pressure along the effective isentrope. If the fluids are in pressure equilibrium, then $p^\alpha = p$ for all α, and

$$
\delta V = \sum_\alpha \delta V^\alpha = -\sum_\alpha \frac{\Delta V^\alpha}{\Gamma^\alpha} \frac{\delta p}{p}\,,
\tag{2.5}
$$

the last equality coming from the requirement that thermodynamic changes in the fluids should keep the fluid in pressure equilibrium if they are initially so, so that δp in (2.5) is independent of α. Comparing (2.4) and (2.5), we obtain

$$\Gamma = \frac{\Delta V}{\sum_\alpha \frac{\Delta V^\alpha}{\Gamma^\alpha}} . \tag{2.6}$$

This Γ is used to calculate the effective Lagrangian sound speed $C^2 = \Gamma p/\tau$. Obtaining the speed of sound in this fashion insures that, at least to leading order in the wave strengths, compressions calculated with the single fluid algorithm are compatible with the assumption that the fluid remains in pressure equilibrium.

Having computed the pressures and velocities at the cell edges with some single fluid Lagrangian algorithm, the specific volumes (equivalently, volumes), total energies of each fluid component and the velocity must be updated. A difference equation for the volume update is obtained from

$$\begin{aligned} \Delta V^{n+1} &= \Delta V^n + \delta V , \\ \delta V &= \Delta t [Au] . \end{aligned} \tag{2.7}$$

The volume of each fluid component is updated by assigning it part of δV:

$$\Delta V^{\alpha,n+1} = \Delta V^{\alpha,n} + \eta^\alpha \delta V \quad , \quad \sum_\alpha \eta^\alpha = 1 . \tag{2.8}$$

By requiring that the changes in the volumes of each of the fluids all correspond to the same pressure change, it must be the case that $(\Delta V^{\alpha,n+1} - \Delta V^{\alpha,n})\,\Gamma^\alpha / \Delta V^{\alpha,n}$ is independent of α. The choice of η^α which uniquely satisfies both the latter requirement and (2.8) is

$$\eta^\alpha = \frac{\Gamma}{\Gamma^\alpha} \frac{\Delta V^{\alpha,n}}{\Delta V^n} . \tag{2.9}$$

It is clear that the total volume is conserved, since $\sum_\alpha \eta^\alpha = 1$. In addition, when Γ^α is a constant independent of α, then $\eta^\alpha = \Delta V^\alpha / \Delta V$ so that the relative compression of each fluid component is the same. This corresponds to the original geometric construction in [17] of letting the subgrid configuration of the fluids expand or contract uniformly, linearly interpolating in volume coordinate the location at any point between the two edges. A major objection to that construction is that fluid components having widely different compressibilities experienced equal relative compressions. The present procedure alleviates that difficulty; for example, if there is one fluid component which is nearly incompressible, then $\Gamma^\alpha \gg \Gamma$ for that fluid, and the other fluid components absorb most of the volume changes.

The velocity equation is quite straightforward, since we only require a single velocity for the cell. It is given by

$$u^{n+1} = u^n + \overline{A}\frac{\Delta t}{\Delta m}[p]\,. \tag{2.10}$$

However, it is useful to notice that this corresponds to a redistribution of the momentum flux difference over n_f momentum equations, one for each fluid, such that the velocity at the new time is independent of α if the velocity at the old time is:

$$u^{n+1,\alpha} = u^{n,\alpha} + \overline{A}\frac{\Delta t}{\Delta m^\alpha}\mu^\alpha[p] \quad , \quad \mu^\alpha = \frac{\Delta m^\alpha}{\Delta m}\,. \tag{2.11}$$

In updating the specific total energies, the energy flux difference is split into two parts: $\frac{1}{2}\overline{Au}\,[p]$, corresponding to the change in the kinetic energy given by the momentum change in (2.11); and $\frac{1}{2}\overline{p}\,[Au]$, corresponding to the work done on the fluid due to the compression or expansion computed from (2.8)–(2.9). Each of these flux differences is distributed over the total energies for each fluid in a manner consistent with the equations (2.8–9) and (2.10):

$$E^{n+1,\alpha} = E^{n,\alpha} + \frac{\Delta t}{\Delta m^\alpha}\left(\frac{1}{2}\overline{Au}\,[p]\,\mu^\alpha + \frac{1}{2}\overline{p}\,[Au]\,\eta^\alpha\right)\,. \tag{2.12}$$

It follows easily that the quantity $E = \sum_\alpha \Delta m^\alpha E^\alpha/\Delta m$ satisfies the conservation law (2.2).

It is clear from the above discussion that, to first order in the local variation of the velocity and pressure, the above algorithm preserves pressure equilibrium between the multifluid components, and that changes in the thermodynamic state of those components are adiabatic if they are in pressure equilibrium. However, it is possible for the various fluid components to develop different pressures due to accumulation of truncation errors, particularly if a large amplitude wave passes through a multifluid cell. For that reason, we provide a mechanism for restoring pressure equilibrium to the components. In doing so, we find a distinguished choice for the function $\hat{p}$ used to calculate the effective pressure in the cell.

At the end of the time step, we compute values for the pressure and sound speed for each fluid using the equation of state, obtaining p^α, Γ^α. We then calculate volume changes

$$\frac{\delta V^\alpha}{\Delta V^\alpha} = \frac{1}{\Gamma^\alpha}\frac{(p^\alpha - \hat{p})}{\hat{p}}\,, \tag{2.13}$$

$$\Delta V^\alpha \leftarrow \Delta V^\alpha + \delta V^\alpha \tag{2.14}$$

which will tend to drive the value of the pressure of the various components of the fluid to $\hat{p}$. The requirement that the total volume of the fluid remain unchanged in this process, i.e., that $\sum_\alpha \delta V^\alpha = 0$ implies that

$$\hat{p} = \sum_\alpha \frac{\Delta V^\alpha p^\alpha}{\Gamma^\alpha} \Big/ \sum_\alpha \frac{\Delta V^\alpha}{\Gamma^\alpha} . \tag{2.15}$$

This is the formula that will be used to compute the average pressure, both here and at the beginning of the time step. In addition, we will also require the energies to change corresponding to the volume changes in (2.14). These are given by

$$\Delta m^\alpha E^\alpha \leftarrow \Delta m^\alpha E^\alpha + \delta E^\alpha , \tag{2.16}$$

$$\delta E^\alpha = -\hat{p}\, \delta V^\alpha . \tag{2.17}$$

Since $\sum_\alpha \delta E^\alpha = 0$, the total energy is also conserved.

3. Eulerian Dynamics.

A system of partial differential equations for which the above procedure constitutes a consistent discretization is developed here. First, an evolution equation for the volume fractions, $f^\alpha = \Delta V^\alpha / \Delta V$, can be derived from (2.7)–(2.9). To do so, notice that

$$\delta(f^\alpha/\rho) = \frac{1}{\rho \Delta V}\, \delta(\Delta V^\alpha) = f^\alpha \frac{\hat{\Gamma}}{\Gamma^\alpha} \frac{[Au]}{\rho \Delta V} \Delta t \tag{3.1}$$

where the fact that $\rho \Delta V$ is an invariant mass increment is used. Making the substitutions $\delta \to \Delta t \frac{\partial}{\partial t}$, $\frac{[\,]}{\rho \Delta V} \to \frac{\partial}{\partial m}$, the Lagrangian equation

$$\frac{\partial}{\partial t}\left(\frac{f^\alpha}{\rho}\right) = f^\alpha \frac{\hat{\Gamma}}{\Gamma^\alpha} \frac{\partial (Au)}{\partial m} \tag{3.2}$$

is obtained.

Similarly, differential equations for the densities ρ^α and total energies $E^\alpha = e^\alpha + u^2/2$ can be derived,

$$\begin{aligned} \frac{\partial}{\partial t}\left(\frac{f^\alpha \rho^\alpha}{\rho}\right) &= 0 , \\ \frac{\partial}{\partial t}\left(\frac{f^\alpha \rho^\alpha E^\alpha}{\rho}\right) &= -p f^\alpha \frac{\hat{\Gamma}}{\Gamma^\alpha} \frac{\partial (Au)}{\partial m} - f^\alpha \frac{\rho^\alpha}{\rho} Au \frac{\partial p}{\partial m} . \end{aligned} \tag{3.3}$$

The momentum equation remains unchanged:

$$\frac{\partial u}{\partial t} + A \frac{\partial p}{\partial m} = 0 . \tag{3.4}$$

In the above equations, $p = \hat{\Gamma} \sum (f^\alpha/\Gamma^\alpha) p^\alpha(\rho^\alpha, e^\alpha)$, $\hat{\Gamma} = (\sum f^\alpha/\Gamma^\alpha)^{-1}$.

These equations extend in a natural way to Eulerian coordinates and multiple dimensions, yielding the following system:

$$\frac{\partial f^\alpha}{\partial t} + \nabla \cdot (\mathbf{u} f^\alpha) = f^\alpha \frac{\hat{\Gamma}}{\Gamma^\alpha} \nabla \cdot \mathbf{u} \tag{3.5a}$$

$$\frac{\partial}{\partial t}(f^\alpha \rho^\alpha) + \nabla \cdot (\mathbf{u} f^\alpha \rho^\alpha) = 0 \tag{3.5b}$$

$$\frac{\partial}{\partial t}(f^\alpha \rho^\alpha E^\alpha) + \nabla \cdot (\mathbf{u} f^\alpha \rho^\alpha E^\alpha) + p f^\alpha \frac{\hat{\Gamma}}{\Gamma^\alpha} \nabla \cdot \mathbf{u} + f^\alpha \frac{\rho^\alpha}{\rho} \mathbf{u} \cdot \nabla p = 0 \tag{3.5c}$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u}\mathbf{u}\rho) + \nabla p = 0\,. \tag{3.5d}$$

These equations can also be derived from a completely formal standpoint, using only the assumptions of conservation of mass, the first law of thermodynamics and the assumption that the fluids are in pressure equilibrium, see Appendix A.

It is easy to show that, if the sum of the f^α's equals 1 initially, then they sum to 1 at all later times. Indeed, if $S = \sum_\alpha f^\alpha$, then it follows from (3.5a) that S satisfies

$$\frac{\partial S}{\partial t} + \mathbf{u} \cdot \nabla S = (1 - S) \nabla \cdot \mathbf{u} \tag{3.6}$$

from which the desired result follows.

By summing the equations for ρ^α, E^α over α, we obtain the usual conservation of mass and energy equations

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0 \\ \frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho \mathbf{u} E + \mathbf{u} p) &= 0\,. \end{aligned} \tag{3.7}$$

Finally, it is easy to show that pressure equilibrium is preserved if it holds initially, i.e., Dp^α/Dt is independent of α if the solution is smooth.

The Eulerian equations (3.5) are used as the basis for deriving our single step Eulerian scheme for multifluid problems. Restricting our attention to one space dimension, the system (3.5) becomes

$$\frac{\partial f^\alpha}{\partial t} + \frac{\partial}{\partial V}(Auf^\alpha) = f^\alpha \frac{\hat{\Gamma}}{\Gamma^\alpha}\frac{\partial Au}{\partial V} \tag{3.8a}$$

$$\frac{\partial \rho^\alpha f^\alpha}{\partial t} + \frac{\partial}{\partial V}(Au\rho^\alpha f^\alpha) = 0 \tag{3.8b}$$

$$\frac{\partial \rho u}{\partial t} + \frac{\partial}{\partial V}(A\rho u^2) + \frac{\partial p}{\partial x} = 0 \tag{3.8c}$$

$$\frac{\partial f^\alpha \rho^\alpha E^\alpha}{\partial t} + \frac{\partial}{\partial V}(Auf^\alpha \rho^\alpha E^\alpha) + f^\alpha p \frac{\hat{\Gamma}}{\Gamma^\alpha}\frac{\partial Au}{\partial V} + \frac{\rho^\alpha f^\alpha}{\rho} Au \frac{\partial p}{\partial V} = 0\,. \tag{3.8d}$$

The remainder of this section is devoted to the development of a discretization for the PDE's (3.8). In the approach taken here, the geometrical construction of subgrid fluid configurations will be confined to the transport of the volume fractions f^α, with the remaining equations differenced using a conservative predictor-corrector formalism. This is in contrast to the technique used in the Lagrange + remap approach, in which the Lagrangian dynamics are computed in a separate Lagrangian calculation, the results of which are averaged conservatively onto the Eulerian mesh. Because the system (3.8) is one-dimensional, the discretization of the advective terms can be performed so that there are no stability problems associated with dividing by $f^{\alpha,n+1}$ in computing the updates of the conserved quantitites. In particular, the mass, momentum, and energy in a cell associated with a particular material are exhausted whenever the volume fraction associated with that material is exhausted. Nevertheless, a redistribution algorithm is needed for the volume fractions and nonadvective parts of the momentum and energy flux differences associated with each material; this is handled in a fashion suggested by equations (2.8), (2.12).

The primary dependent variables for the discrete solution are given by u_j^n, $f_j^{\alpha,n}$, $\rho_j^{\alpha,n}$, $E_j^{\alpha,n}$, the velocity of the fluid in the cell, and the volume fraction, density, and specific total energy for each fluid in the cell, where the latter two variables are defined only for those j, α with $f_j^{\alpha,n} > 0$. Given these quantities, the various derived quantities such as internal energy, pressure, and sound speed Γ for each fluid are given as in the Lagrangian case.

The overall time-stepping strategy is analogous to that used in the Lagrangian case. A single fluid algorithm for (3.5d), (3.7) is used to calculate the effective compressible dynamics of the multicomponent fluid, and then each fluid component is evolved separately in a thermodynamically consistent fashion. The underlying single fluid algorithm is the second-order Godunov method [6], as described in [4] for a general equation–of–state. This

algorithm requires as input p_j^n, u_j^n, E_j^n, values for the conserved quantities, as well as values for the derived quantitites p_j^n, γ_j^n, Γ_j^n. These are given as follows:

$$
\begin{aligned}
\rho^n &= \sum_\alpha f^{\alpha,n}\rho^{\alpha,n} \\
\Gamma^n &= \left(\sum_\alpha \frac{f^{\alpha,n}}{\Gamma^{\alpha,n}}\right)^{-1} \\
p^n &= \Gamma^n \sum_\alpha \left(\frac{f^{\alpha,n}p^{\alpha,n}}{\Gamma^{\alpha,n}}\right) \\
E^n &= \left(\sum f^{\alpha,n}\rho^{\alpha,n}E^{\alpha,n}\right) \Big/ \rho^n \\
e^n &= E^n - \frac{(u^n)^2}{2} \\
\gamma^n &= \frac{p^n}{\rho^n e^n} + 1\,.
\end{aligned}
\tag{3.9}
$$

There are two sets of information required from the single fluid algorithm. First, the multimaterial algorithm must reduce to it for the single fluid case in the sense that it provides the fluxes for cells which both are single fluid cells and have only single fluid cells on either side of them; in particular, we require the time–centered quantities $q = p$, u, ρ, e at cell edges. Second, these quantities may also be needed for cell edges adjacent to a multifluid cell, see equations (3.14), (3.15) below; and the time-centered values of $q_{j+1/2}$, $q = p$, u are always needed to update multifluid quantities. A single fluid algorithm satisfying these properties is presented in Appendix B and was used to obtain our numerical results.

The discretization of (3.8a), i.e., the finite difference approximation of the evolution of the volume fractions f^α on the Eulerian grid, is a key step in transferring the ideas of Section 2 to the Eulerian context. First, an algorithm is presented which is sufficient for virtually any problem for which all the fluids are gases. Afterwards, a correction for the general case is constructed.

The calculation for the basic algorithm proceeds in two steps. First, the left hand side of (3.8a) is approximated by a conservative difference, which is given by

$$
\tilde{f}^\alpha = f^{\alpha,n} + \frac{1}{\Delta V}[\Delta V^{\alpha,\mathrm{slic}}] \tag{3.10}
$$

where $\Delta V_{j+1/2}^{\alpha,\mathrm{slic}}$ is the (signed) volume of fluid α which will cross the cell interface at $x = x_{j+1/2}$ during the time step, assuming that the right hand side of (3.8a) is zero and the subgrid configuration of the fluid volumes is given by the SLIC construction in [11]; Appendix C outlines our implementation in the present context of computing provisional volume fraction updates. For example, contained between $x_{j+1/2}$ and $x_{j+1/2} - u_{j+1/2}\,\Delta t$,

where the subgrid configuration of the fluid volumes is given by the SLIC construction in [11], see Appendix C for an outline of our implementation. If we define $V^{\rm tot}_{j+1/2} = V(x_{j+1/2}) - V(x_{j+1/2} - u_{j+1/2}\Delta t)$, then $V^{\rm tot}_{j+1/2} \sim (Au)_{j+1/2}\Delta t$, and $\Delta V^{\alpha,{\rm slic}} \sim f^{\alpha}_{j+1/2} \cdot V^{\rm tot}_{j+1/2}$, so that (3.10) constitutes a formally consistent discretization of the left hand side of (3.8a).

The second step is to calculate the effect of the right hand side of (3.8a) on $\tilde{f}^{\alpha}$ to obtain $f^{\alpha,n+1}$. It follows from (3.10) and the ensuing discussion that

$$Du = \frac{1}{\Delta t}\left(1 - \sum_{\alpha} \tilde{f}^{\alpha}\right) \tag{3.11}$$

approximates $\partial(Au)/\partial V$. Therefore, $f^{\alpha,n+1}$ is set to be

$$f^{\alpha,n+1} = \tilde{f}^{\alpha}\left(1 + \frac{\hat{\Gamma}}{\tilde{\Gamma}^{\alpha}}\Delta t\,(Du)\right), \tag{3.12}$$

where

$$\tilde{\Gamma}^{\alpha}_{j} = \frac{\sum_{s=0,\pm 1} f^{\alpha,n}_{j+s}\,\Gamma^{\alpha,n}_{j+s}}{\sum_{s=0,\pm 1} f^{\alpha,n}_{j+s}} \tag{3.13a}$$

and

$$\hat{\Gamma} = \left(\sum_{\alpha} \frac{\tilde{f}^{\alpha}}{\tilde{\Gamma}^{\alpha}}\right)^{-1}. \tag{3.13b}$$

This discretization has the property that $1 \geq f^{\alpha,n+1} \geq 0$ and $\sum_{\alpha} f^{\alpha,n+1} = 1$. In particular, if all the $\tilde{\Gamma}^{\alpha}$'s are equal, the second step in the procedure corresponds to normalizing each of the $\tilde{f}^{\alpha}$'s by $\sum_{\alpha} \tilde{f}^{\alpha}$.

The algorithm given by (3.10)–(3.13) can fail in practice. Indeed, let $n_f = 2$ and suppose that $\rho^1_j \gg \rho^2_j$ where the jth zone is the interface between two fluids. If $\Delta V^{2,{\rm slic}}_{j+\frac{1}{2}} > f^2_j$ and $u_{j+\frac{1}{2}} > 0$ then it follows that the light fluid leaves the jth zone entirely. If also the Riemann problem at the (j-1)-interface does not lead to enough (or any) of the heavy fluid entering the jth zone, then the resultant heavy fluid is forced to expand to fill the zone in accord with (3.11)–(3.13). For a stiff EOS, this can easily force the fluid into regions for which the EOS is invalid and the calculation either collapses or is meaningless. The situation described occurs, for example, if air moves away from an air/water interface due to a rarefaction wave.

It is easy to see that this failure of the algorithm is an artifact of computing in Eulerian coordinates and not taking into appropriate account the effective Lagrangian dynamics

(see the discussion following (2.9)) in computing interface volume fluxes. A resolution is obtained by performing the calculation of $\Delta V^{\alpha,\mathrm{slic}}_{j+\frac{1}{2}}$ in Lagrangian coordinates instead when necessary along with a treatment of the relative expansions at the interface which is exactly analogous to (3.11)–(3.13); note that the extra steps described here can be entirely eliminated for many applications, e.g., for problems involving only gases.

Therefore, the following computations are performed *prior* to steps (3.10)–(3.13). First, define

$$\Delta V^{\mathrm{Lag}} = \Delta V + \Delta t[Au]\,. \tag{3.14}$$

If $\Delta V^{\mathrm{Lag}} \leq \Delta V$, then the zone is compressing and there are no numerical difficulties in practice. Otherwise, $\Delta V^{\mathrm{Lag}} > \Delta V$ and the zone is expanding. Then, each fluid is expanded into the larger volume ΔV^{Lag}, i.e.,

$$\tilde{f}^{\alpha} = f^{\alpha,n}\frac{\Delta V}{\Delta V^{\mathrm{Lag}}}\,. \tag{3.15}$$

Next, the quantities $\tilde{f}^{\alpha}$ from (3.15) are used to compute Du, $\tilde{\Gamma}^{\alpha}$, $\hat{\Gamma}$ by direct analogy to (3.11), (3.13a) and (3.13b), respectively. The update

$$\tilde{f}^{\alpha} \leftarrow \tilde{f}^{\alpha}\left(1 + \frac{\hat{\Gamma}}{\tilde{\Gamma}^{\alpha}}\Delta t\,(Du)\right) \tag{3.16}$$

is made in analogy to (3.12) and the partial volumes

$$\Delta\tilde{V}^{\alpha} = \tilde{f}^{\alpha}\Delta V^{\mathrm{Lag}} \tag{3.17}$$

are computed. The quantities ΔV^{Lag} and $\Delta\tilde{V}^{\alpha}$ are then used in place of ΔV and ΔV^{α} in the SLIC computation described in Appendix C. The resulting 'Lagrangian' volume fluxes must then be recalibrated for the Eulerian scheme as folows:

$$\Delta V^{\alpha,\mathrm{slic}} \leftarrow V^{\alpha,\mathrm{slic}} f^{\alpha,n}\frac{\Delta V}{\Delta\tilde{V}^{\alpha}}\,. \tag{3.18}$$

The update of the remaining conserved quantities uses a standard conservative differencing of (3.8b)–(3.8d) which reduces to the single fluid differencing away from fluid interfaces. Define $q^{ad}_{j+1/2}$, $q = \rho^{\alpha}$, e^{α}, u to be q^{n}_{j} if the streamline from the cell center defined by $u_{j+1/2}$ traces back into a cell containing more than one material; otherwise, it is the value obtained from the single fluid calculation. Also, define the auxiliary quantities

$$\begin{aligned}
M^{\rho,\alpha}_{j+1/2} &= V^{\alpha,\mathrm{slic}}_{j+1/2}\rho^{\alpha,ad}_{j+1/2}\,,\\
M^{\rho u}_{j+1/2} &= \left(\sum_{\alpha} M^{\rho,\alpha}_{j+1/2}\right) u^{ad}_{j+1/2}\,,\\
M^{\rho E,\alpha}_{j+1/2} &= M^{\rho,\alpha}_{j+1/2}\left(e^{ad}_{j+1/2} + \frac{1}{2}(u^{ad}_{j+1/2})^2\right)\,.
\end{aligned} \tag{3.19}$$

The update of the conserved quantities is then given by the following difference equations:

$$
\begin{aligned}
(f^\alpha \rho^\alpha)^{n+1} &= (f^\alpha \rho^\alpha)^n + \frac{1}{\Delta V}[M^{\rho,\alpha}] \\
\rho^{n+1} &= \sum_\alpha (f^\alpha \rho^\alpha)^{n+1} \\
(\rho u)^{n+1} &= (\rho u)^n + \frac{1}{\Delta V}[M^{\rho u}] + \frac{\Delta t}{\Delta x}[p] \\
(f^\alpha \rho^\alpha E^\alpha)^{n+1} &= (f^\alpha \rho^\alpha E^\alpha)^n + \frac{1}{\Delta V}[M^{\rho E,\alpha}] \\
&\quad + f^{\alpha,n+1}\frac{\Delta t}{\Delta V}(\overline{p}\,\frac{\hat{\Gamma}}{\tilde{\Gamma}^\alpha}[Au] + \frac{\rho^{\alpha,n+1}}{\rho^{n+1}}\,\overline{Au}\,[p]\,).
\end{aligned}
\tag{3.20}
$$

Once the conserved quantitites have been updated, it is still necessary to perform the relaxation scheme (2.13)–(2.17) to maintain pressure equilibrium in the multifluid cells. This is implemented for our Eulerian system by calling the EOS for each fluid using the updated multifluid values as input, calculating $\hat{p}$ from (2.15) and the new values of p^α, using (2.13) to obtain the volume fraction changes δf^α and then calculating

$$
\begin{aligned}
f^{\alpha,n+1} &\leftarrow f^{\alpha,old} + \delta f^\alpha \\
\rho^{\alpha,n+1} &\leftarrow \rho^{\alpha,n+1}\frac{f^{\alpha,old}}{f^{\alpha,n+1}} \\
E^{\alpha,n+1} &\leftarrow (f^{\alpha,old}E^{\alpha,n+1} - \hat{p}\,\delta f^\alpha)/f^{\alpha,n+1}
\end{aligned}
\tag{3.21}
$$

where $f^{\alpha,old}$ is the value of $f^{\alpha,n+1}$ just after (3.20) is computed.

In practice, δf^α may be replaced by $\sigma \cdot \delta f^\alpha$ in the above calculation for any value of σ in the range $0 \le \sigma \le 1$. For the calculations of Section 4, the value $\sigma = 0.95$ is used.

Up to this point, our method is directly applicable to problems in which a material pressure becomes negative (of course, sound speeds are calculated using the absolute value of the pressure). An example is (even slightly) overexpanded water. For general multimaterial calculations, such examples occur frequently since heavy materials with stiff EOS's will be dynamically interacting with air and similar materials. The results to be presented in the next section involve a situation for which it is difficult to make sense of (2.13)–(2.17); therefore, (3.21) is not implemented if a negative pressure is present at a cell edge. In other examples, it is possible to replace a (negative) material pressure by its absolute value and proceed with (3.21).

4. Computational Results.

The numerical method developed in Section 3 and Appendices B and C has already been extensively used in studies of shock wave refractions and other problems. The reader is referred to [5], [10], [12], [19] and [21] for the work on shock wave refraction in gases. Recently, a variant of the scheme has also been applied to problems involving water and

(heavy, i.e., initial densities of order unity) air (and/or other gases), see [24]. All of these papers describe results from codes based on operator split implementations of the algorithm of Section 3, just as we do here.

Our method has been further extended to three space dimensions with adaptive mesh refinement (AMR) capability in [23]. This paper also introduces an alternative (better(???), but still first–order) interface reconstruction algorithm. A second–order accurate interface reconstruction algorithm has recently been introduced, see [18], and applied to shock wave refractions in gases [11], [13], [14], [22].

The EOS for air is taken to be the standard polytropic model $p = (\gamma - 1)\rho e$. For water, the calculation uses the Tait EOS:

$$\begin{aligned} \frac{p}{p_0} &= A(\frac{\rho}{\rho_0})^7 - B \\ c^2 &= 7A(\frac{\rho}{\rho_0})(\frac{\rho}{\rho_0})^6 \end{aligned} \tag{4.}$$

where A = 3001, B = 3000 and $(\rho_0, p_0) = (0.99821, 1.01325e+06)$ in cgs units. Note that $p_0 = 1$ atmosphere.

The computational domain for this calculation is $D = \{x : 0 \leq x \leq 1000\}$. The right half of D consists of ambient water with $(\rho, p) = (\rho_0, p_0)$ as above. The air is initially given by $\mathbf{u}_M = (\rho_M, p_M, u_M) = (1.223e-03, 1\,\text{atm}, 0)$ in the region $D_M = \{x : 400 \leq x \leq 500\}$, and $\mathbf{u}_L = (\rho_L, p_L, u_L) = (,,)$. Here, $\mathbf{u}_L$ is precomputed so that the states $(\mathbf{u}_L, \mathbf{u}_M)$ are connected by a forward–facing rarefaction wave in phase space.

The computational domain is $D = \{(x, y) : 0 \leq x \leq 150, 0 \leq y \leq 37.5\}$; where here and below distance is measured in meters for convenience. Initially, a contact surface separates a region of SF_6 which is modelled here as a perfect gas with $\gamma = 1.18$ and a region of air. The former region is given by $D_{SF_6} = \{x : 50 \leq x \leq 150, 0 \leq y \leq 18.75\}$ and D_{air} is its complement in D. The initial data in D_{SF_6} is given everywhere by $(\rho, u, p) = (4.892e-03, 0, 1\,\text{atm}$; in D_{air}, a planar forward–facing shock wave with shock wave Mach number $M_s = 1.7$ is situated at $x = 22.5$. Ahead of the shock, the initial data in D_{air} is given everywhere by $(\rho, u, p) = (1.223e-03, 0, 1\,\text{atm})$ and the initial state in the region behind the shock is calculated from the Rankine–Hugoniot conditions.

5. Conclusions.

Appendix A
Derivation of the Multifluid Differential Equations

In this section, a formal derivation of equations (3.8) is presented, along with a proof that these equations form a hyperbolic system in which the constraint of pressure equilibrium appears as an initial value constraint. The starting point for this derivation is the following set of assumptions about the system:

(1) Conservation of mass for each fluid component:

$$\frac{D}{Dt}(f^\alpha \rho^\alpha) + f^\alpha \rho^\alpha \nabla \cdot \mathbf{u} = 0 \ , \ \alpha = 1, \ldots, n_f \, . \tag{A.1}$$

(2) Changes of state for each fluid component are adiabatic:

$$\frac{De^\alpha}{Dt} + p^\alpha \frac{D}{Dt}(\frac{1}{\rho^\alpha}) = 0 \ , \ \alpha = 1, \ldots, n_f \tag{A.2}$$

where $p^\alpha = p^\alpha(\rho^\alpha, e^\alpha)$.

(3) Pressure equilibrium among components, i.e., there is a function $p(x,t)$ such that

$$p^\alpha(x,t) = p(x,t) \ , \ \alpha = 1, \ldots, n_f \, . \tag{A.3}$$

(4) A single momentum equation holds for the fluid mixture:

$$\frac{D\mathbf{u}}{Dt} + \frac{1}{\rho}\nabla p = 0 \, , \tag{A.4}$$

where the mean density $\rho = \sum_\alpha f^\alpha \rho^\alpha$.

(5) The fluid components fill the available volume:

$$\sum_\alpha f^\alpha = 1 \, . \tag{A.5}$$

These equations constitute a set of $3n_f + d + 1$ equations for the same number of unknowns $(\{\rho^\alpha, e^\alpha, f^\alpha; \alpha = 1, \ldots, n_f\}, \mathbf{u}, p)$, where d is the number of space dimensions.

To derive the equations (3.8), a series of transformations on (A.1) - (A.5) are performed. First, notice that (A.2) and (A.3) lead to a set of evolution equations for ρ^α:

$$\frac{1}{\rho^\alpha}\frac{D\rho^\alpha}{Dt} = \frac{1}{p^\alpha \Gamma^\alpha}\frac{Dp^\alpha}{Dt} = \frac{1}{p\Gamma^\alpha}\frac{Dp}{Dt} \, . \tag{A.6}$$

Using conservation of mass for each fluid component and (A.6), the following evolution equation for f^α is obtained:

$$\frac{Df^\alpha}{Dt} + f^\alpha \nabla \cdot \mathbf{u} + \frac{f^\alpha}{p\Gamma^\alpha}\frac{Dp}{Dt} = 0 \, . \tag{A.7}$$

Summing over α and using (A.5) leads to

$$\frac{Dp}{Dt} + \hat{\Gamma} p \nabla \cdot \mathbf{u} = 0 \, , \; \hat{\Gamma} = \left(\sum_{\alpha} \frac{f^{\alpha}}{\Gamma^{\alpha}} \right)^{-1} . \tag{A.8}$$

Using (A.8), we obtain the following system of equations for our dependent variables:

$$\begin{aligned}
&\frac{Df^{\alpha}}{Dt} + f^{\alpha} \left(1 - \frac{\hat{\Gamma}}{\Gamma^{\alpha}} \right) \nabla \cdot \mathbf{u} = 0 \\
&\frac{D\rho^{\alpha}}{Dt} + \rho^{\alpha} \frac{\hat{\Gamma}}{\Gamma^{\alpha}} \nabla \cdot \mathbf{u} = 0 \\
&\frac{De^{\alpha}}{Dt} + \frac{p^{\alpha}}{\rho^{\alpha}} \frac{\hat{\Gamma}}{\Gamma^{\alpha}} \nabla \cdot \mathbf{u} = 0 \\
&\frac{Dp}{Dt} + p \hat{\Gamma} \nabla \cdot \mathbf{u} = 0 \\
&\frac{D\mathbf{u}}{Dt} + \frac{1}{\rho} \nabla p = 0 \, .
\end{aligned} \tag{A.9}$$

We note that, if we take the system (A.9) as given, we can derive the equations (A.1) - (A.5), with the constraints (A.3) and and (A.5) as initial value constraints. The evolution equation for $S = \sum_{\alpha} f^{\alpha}$ obtained from summing the equations for f^{α} over α is $DS/Dt = (1 - S) \nabla \cdot \mathbf{u}$ (see (3.6)), so that $S = 1$ for all time if $S(x, 0) = 1$. Similarly, the equations for $\rho^{\alpha}, e^{\alpha}, p$ imply (A.6) which, in turn, implies that

$$\frac{D \log p^{\alpha}}{Dt} = \frac{D \log p}{Dt} \, , \; \alpha = 1, \ldots, n_f \, , \tag{A.10}$$

and $p^{\alpha} = p$ for all time if $p^{\alpha}(x, 0) = p(x, 0)$, independent of α. In particular, we may replace p^{α} by p in the equation for e^{α}. Equivalently, the equation for p is redundant, since we can replace it with any of the p^{α} computed from $\rho^{\alpha}, e^{\alpha}$ and the appropriate equation of state, or any average of the p^{α}'s. Starting with equations (A.9), it is routine to derive the system (3.8).

To show that the system (A.9) is hyperbolic, we need only consider the case of variation in one space dimension. In that case, the dependent variables are $Q = (\{f^{\alpha}, \rho^{\alpha}, e^{\alpha}, \alpha = 1, \ldots, n_f\}; u, p)^t$, where without loss of generality we have only kept the normal velocity component. In that case, (A.9) can be written in the form

$$Q_t + A Q_x = 0 \tag{A.11}$$

$$A - uI = \begin{pmatrix} & & & 0 & \\ & \mathcal{O} & & \vdots & \mathbf{b} \\ & & & 0 & \\ 0 & \cdots & 0 & 0 & p\hat{\Gamma} \\ 0 & \cdots & 0 & \frac{1}{\rho} & 0 \end{pmatrix} , \tag{A.12}$$

with $\mathbf{b} = (1 - \frac{\hat{\Gamma}}{\Gamma^\alpha}\frac{\rho^\alpha}{\rho}, \rho^\alpha \frac{\hat{\Gamma}}{\Gamma^\alpha}, \frac{\rho\hat{\Gamma}}{\rho^\alpha\Gamma^\alpha}, \alpha = 1, \ldots, n_f)^t$. The characteristic polynomial for A is given by $\det(\lambda I - A) = (\lambda - u)^{3n_f}((\lambda - u)^2 - p\hat{\Gamma}/\rho)$. Therefore, the eigenvalues of A are given by $\lambda = u \pm c, c^2 = p\hat{\Gamma}/\rho$ and $\lambda = u$ (with multiplicity $3n_f$). In addition, a complete set of right eigenvectors can be constructed.

A physical interpretation of the eigenstructure is that the system (A.9) supports two compressive modes moving relative to the fluid at an effective sound speed for the mixture, and $3n_f$ modes carrying variations in the multifluid properties along particle paths. Finally, we note that there are both similarities and differences between the situation here and that for the equations describing multiphase mixtures in porous media flow [1]. In both cases, the constraint (A.5) is used to derive an evolution equation for a common thermodynamic pressure for the mixture. In the porous media case, differentiating the constraint equation in time, combined with D'Arcy's law, leads to an elliptic or parabolic equation for the pressure; in the present case, differentiating the constraint equation along particle paths leads to the hyperbolic system (A.9), with the constraint equations (A.3) and (A.5) on the pressure and volume fractions appearing as initial value constraints.

Appendix B
A Single Fluid Eulerian Godunov Scheme for a General Equation–of–State

In this appendix, a second–order Godunov method for compressible flow in one space dimension for a fluid with an arbitrary (convex) equation–of–state is developed; the equations to be discretized are:

$$\frac{\partial U}{\partial t} + \frac{\partial AF(U)}{\partial V} + \frac{\partial H(U)}{\partial x} = 0\,, \tag{B.1}$$

Here $V = V(x)$ is a generalized volume coordinate, with $A = A(x) = \frac{dV}{dx} > 0$ the cross-sectional area associated with $V(x)$. The conserved quantities and fluxes are given by

$$U = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \end{pmatrix}\,,\ F(U) = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uE + up \end{pmatrix}\,,\ H(U) = \begin{pmatrix} 0 \\ p \\ 0 \\ 0 \end{pmatrix}$$

where ρ is the density, u the velocity in the x–direction, v the tranverse velocity, E the total energy per unit mass, and p the pressure obtained from the equation of state: $p = p(\rho, e)$, $e = E - \frac{u^2+v^2}{2}$.

Let $\{x_{j+\frac{1}{2}}\}$ be the edges of a finite difference mesh, and Δt a time increment. Conservative finite difference approximations of the form

$$U_j^{n+1} = U_j^n + \frac{\Delta t}{\Delta V_j}(A_{j-\frac{1}{2}}F_{j-\frac{1}{2}} - A_{j+\frac{1}{2}}F_{j+\frac{1}{2}}) + \frac{\Delta t}{\Delta x_j}(H_{j-\frac{1}{2}} - H_{j+\frac{1}{2}}) \tag{B.2}$$

are considered, where $\Delta x_j = x_{j+\frac{1}{2}} - x_{j+\frac{1}{2}}$, $\Delta V_j = V(x_{j+\frac{1}{2}}) - V(x_{j-\frac{1}{2}})$, $A_{j+\frac{1}{2}} = A(x_{j+\frac{1}{2}})$ and $F_{j+\frac{1}{2}}$, $H_{j+\frac{1}{2}}$ are some approximation of the time averages of F and H at $x_{j+\frac{1}{2}}$. The strategy for computing $F_{j+\frac{1}{2}}$, $H_{j+\frac{1}{2}}$ follows the general predictor–corrector formalism in [4], [6], [7].

In the formulation of the predictor step, a convenient set of characteristic variables Q satisfying the property that that $Q = Q(U)$ is an invertible function of U is required. The equations (B.1) then transform into the quasilinear form

$$\frac{\partial Q}{\partial t} + \mathbf{A}(Q)\frac{\partial Q}{\partial x} = G(Q, x)\,. \tag{B.3}$$

The matrix $\mathbf{A}$ has real eigenvalues $\lambda_1 < \ldots < \lambda_N$ with associated biorthogonal right and left eigenvectors $\{r_k\}, \{l_k\}, k = 1, \ldots, N$.

The prediction of time–centered left and right states at the cell interfaces follows the general strategy of [4] and is given as follows:

$$\begin{aligned} Q_{j+\frac{1}{2},L} &= Q_j^n + \frac{\Delta t}{2}G_j^n + \frac{1}{2}P_+(I - A(Q_j^n)\frac{\Delta t}{\Delta x_j})\Delta Q_j\,, \\ Q_{j+\frac{1}{2},R} &= Q_{j+1}^n - \frac{\Delta t}{2}G_{j+1}^n + \frac{1}{2}P_-(I + A(Q_{j+1}^n)\frac{\Delta t}{\Delta x_j})\Delta Q_{j+1}\,. \end{aligned} \tag{B.4}$$

Here, the slopes ΔQ_j are a finite difference approximation to $\frac{\partial Q}{\partial x}\Delta x_j$ to which monotonicity constraints have been applied, in the same fashion as for the explicit second-order Godunov methods in [4], [6]. The projection operators $P_\pm$ are defined by

$$P_+ w = \sum_{\{\lambda_k : \lambda_k > 0\}} (l_k \cdot w) r_k \ , \ P_- w = \sum_{\{\lambda_k : \lambda_k < 0\}} (l_k \cdot w) r_k \ .$$

To complete the description of the predictor step, an approximate Riemann problem solver which leads to a mapping $(Q_{j+\frac{1}{2},L}, Q_{j+\frac{1}{2},R}) \rightarrow Q_{j+\frac{1}{2}}$ is required. For the present purpose of computing single fluid fluxes in an explicit multifluid algorithm, this mapping is defined by using the Godunov state of the approximate Riemann problem solution. See [7] for the construction of a similar approximate Riemann problem solver which is used in conjunction with the Engquist–Osher flux formula.

An important design principle of efficient Godunov-like algorithms is that multiple evaluations of the EOS in a time step are to be avoided. To accomplish this, the dimension of Q is greater than the dimension of U. These redundant variables are chosen in such a way that the entire flux vector can be computed as a simple algebraic function of Q without calling the EOS. In [4] the augmented characteristic variables are $Q = (\rho, u, p, v, \gamma)^t$, where γ is defined by $\gamma = p/(\rho e) + 1$ wheras the variables $Q = (\rho, u, p, v, \rho e)^t$ have been chosen for the present work. Also, the approximate Riemann problem solver of [4] is replaced by a considerably simplified version, in the spirit of the BCT formulation [1]. The net result is an algorithm which is twice as fast as the one in [4] and somewhat easier to program. Additionally, this new algorithm is more generally applicable than the older version which was really designed around equations–of–state for real gases, for which γ is well–defined thermodynamically. In particular, neither p nor e are required to be positive for the present algorithm to work.

Explicitly, the characteristic equations (B.3) are:

$$\begin{aligned}
&\frac{D\rho}{Dt} + \rho\frac{\partial u}{\partial x} = -\frac{A'}{A}\rho u \\
&\frac{Du}{Dt} + \frac{1}{\rho}\frac{\partial p}{\partial x} = 0 \\
&\frac{Dp}{Dt} + \rho c^2\frac{\partial u}{\partial x} = -\frac{A'}{A}\rho u c^2 \\
&\frac{Dv}{Dt} = 0 \\
&\frac{D(\rho e)}{Dt} + \rho i\frac{\partial u}{\partial x} = -\frac{A'}{A}\rho i u \, ,
\end{aligned} \tag{B.5}$$

where $i = e + p/\rho$ is the specific internal enthalpy. It is easy to check that the eigenvalues of the characteristic matrix $\mathbf{A}$ are given by $\lambda = \{u - c, u, u, u, u + c\}$, the matrix of right

eigenvectors is

$$R = \begin{pmatrix} 1 & 0 & 1 & 0 & 1 \\ -\tau c & 0 & 0 & 0 & \tau c \\ c^2 & 0 & 0 & 0 & c^2 \\ 0 & 1 & 0 & 0 & 0 \\ i & 0 & 0 & 1 & i \end{pmatrix} \tag{B.6}$$

where $\tau = \rho^{-1}$, and the corresponding matrix of left eigenvectors is

$$L = \begin{pmatrix} 0 & -\frac{\rho}{2c} & \frac{1}{2c^2} & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & -\frac{1}{c^2} & 0 & 0 \\ 0 & 0 & -\frac{i}{c^2} & 0 & 1 \\ 0 & \frac{\rho}{2c} & \frac{1}{2c^2} & 0 & 0 \end{pmatrix} . \tag{B.7}$$

The Riemann problem solver begins with the calculation of (p^*, u^*) by linearization:

$$\begin{aligned} p^* &= \frac{W_R p_L + W_L p_R + W_L W_R (u_L - u_R)}{W_L + W_R} \\ u^* &= \frac{W_L u_L + W_R u_R + p_L - p_R}{W_L + W_R} , \end{aligned} \tag{B.8}$$

where $W^2_{L,R} = (\Gamma \rho p)_{L,R}, \Gamma = \rho c^2/p, \Gamma_{L,R} = \Gamma(U^n_{j,j+1})$. Setting $c^2_{L,R} = (\Gamma p/\rho)_{L,R}$, the remainder of the $*$–state calculation proceeds as follows:

$$\begin{aligned} \rho^*_{L,R} &= \rho_{L,R} + \frac{p^* - p_{L,R}}{c^2_{L,R}} , \\ (c^*_{L,R})^2 &= \Gamma_{L,R} p^* / \rho^*_{L,R} , \\ (\rho e)^*_{L,R} &= (\rho e)_{L,R} + (p^* - p_{L,R})(\frac{i}{c^2})_{L,R} , \\ v^*_{L,R} &= v_{L,R} . \end{aligned} \tag{B.9}$$

For equations–of–state for which there is a possibility that the pressure p may change sign, absolute values of c^2 are taken prior to obtaining c from the square root.

The (approximate) Godunov state Q_G is defined to be the value of Q along the ray $x/t = 0$ and is computed in two steps. First, we set

$$Q, Q^* = \begin{cases} Q_L, Q^*_L , \text{if } u^* > 0 \\ Q_R, Q^*_R , \text{otherwise} , \end{cases} \tag{B.10a}$$

and

$$\lambda, \lambda^* = c - su, c^* - su^* \tag{B.10b}$$

where $s = \mathrm{sgn}(u^*)$. Also, an approximate shock speed

$$\sigma = \frac{1}{2}(\lambda + \lambda^*) \tag{B.10c}$$

is computed. Second, if $\lambda^* > \lambda$, then

$$Q_G = \begin{cases} Q\,, \text{ if } \sigma < 0 \\ Q^*, \text{ otherwise}\,; \end{cases} \tag{B.11a}$$

otherwise, if $\lambda^* < \lambda$, then

$$Q_G = \begin{cases} Q\,, \text{ if } \lambda < 0 \\ Q^*\,, \text{ if } \lambda^* > 0 \\ \alpha Q^* + (1-\alpha)Q\,, \text{ otherwise}\,. \end{cases} \tag{B.11b}$$

Here, $\alpha = \frac{1}{2}(1 + \frac{\lambda+\lambda^*}{\lambda-\lambda^*})$. These two steps guarantee entropy–satisfying waves; the last equation implements linear interpolation in the wave speed to approximate the solution inside a rarefaction fan.

Finally, the fluxes are evaluated from the time–centered states $Q_{j+\frac{1}{2}}$ as follows:

$$F_{j+\frac{1}{2}} = \begin{pmatrix} \rho_{j+\frac{1}{2}} u_{j+\frac{1}{2}} \\ \rho_{j+\frac{1}{2}} u^2_{j+\frac{1}{2}} \\ \rho_{j+\frac{1}{2}} u_{j+\frac{1}{2}} v_{j+\frac{1}{2}} \\ ((\rho e)_{j+\frac{1}{2}} + \frac{1}{2}\rho_{j+\frac{1}{2}} u^2_{j+\frac{1}{2}}) u_{j+\frac{1}{2}} + u_{j+\frac{1}{2}} p_{j+\frac{1}{2}} \end{pmatrix}. \tag{B.12}$$

To summarize, the single fluid algorithm consists of the following four steps: (1) monotonized slopes ΔQ_j are computed for an augmented state vector Q associated with a convenient transformed system (B.3); (2) the projection operators are applied to construct time-centered left and right states (B.4); (3) the approximate Riemann problem solver described in this section resolves nonlinear wave interactions at interfaces and the Godunov state is used as the interface state $Q_{j+\frac{1}{2}}$; and (4) fluxes are evaluated at these interface states, (B.12), and the general explicit conservative update formula (B.2) is calculated.

Appendix C
Subgrid Multifluid Representation Using SLIC

The SLIC (Simple Line Interface Calculation) algorithm [11] is a procedure for representing the subgrid structure of multifluid zones based on local volume-of-fluid information. This information is used to advect fluid volume fractions, see (3.10), and it is essential that the construction leads to appropriate global interface movements. Indeed, a noteworthy aspect of this work is that the multifluid algorithm coupled with the SLIC construction is capable of achieving this goal using only a local interface reconstruction. SLIC and related volume-of-fluid constructions have been widely used in compressible flow codes as well as in other areas of fluid mechanics, e.g., flame front propagation [9], Hele–Shaw interfaces [25], astrophysical jets [26] and the references discussed in Section 4.

Since its introduction, SLIC has been adapted and modified by several groups. We present here our 1D split version which has been used for the calculations herein. This version is very close to the original [11]; in particular, the subgrid construction is restricted to horizontal and vertical lines. The reader is referred to [18] where SLIC and newer first-order as well as second-order reconstruction algorithms are compared (for accuracy) in the context of linear advection.

The construction of multifluid geometric structure in the jth zone is a function of the data $\{\Delta V^{\alpha}_{j+s} : s = \pm 1, 0\,; \alpha = 1, \ldots, n_f\}$. Figure C1 illustrates the possible results of the SLIC calculation as implemented here for the case of two fluids. Here, it is assumed that the jth zone is nontrivially multifluid (i.e., contains nonzero amounts of both 'black' and 'white' fluid). Of course, the extent of the black shading in each of these configurations will correspond exactly to the volume fractions in the jth zone. On the other hand, there is no cutoff in determining the type (that is, all white, all black or black and white) of the zones to the left and right, so that a zone will be treated as 'black and white' unless one of the volume fractions is close (i.e., a few orders of magnitude greater than) to machine roundoff. A simple smooth interface, overlayed on a square grid, is illustrated in Figure C2 along with its' SLIC reconstruction as it would be calculated in a fractional step of the overall algorithm in the x–direction (assuming that the initial volume fractions are in accord with the figure).

The case in which, say, 'black' fluid is between two 'all white' zones is a little trickier. In a two–dimensional context, this situation can arise if a long, thin 'black' region is situated transverse to the current sweep direction. The naive approach for this case is to center the 'black' fluid in the zone. However, consider a problem for which the local fluid (hence, interface) velocity is significantly less than the (global) maximum wave speed used to compute the CFL number and the time step. It is then possible that no 'black' fluid will ever cross the zone interface in the flow direction. Thus, a more robust approach is required. Our implementation of SLIC uses a 'random choice' technique; the 'left' and 'right' interfaces of the 'black' fluid are placed randomly and with equal probability in the zone subject only to the obvious constraint that the entire 'black' region must be contained

in the zone.

It is not obvious that a multidimensional interface will remain recognizable after several time steps. Indeed, if the interface is physically unstable then this is not even desirable.

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